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Improved Control Strategies for Atomic Force Microscopes in Intermittent Contact Mode

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Abstract—Atomic force microscopes have proved to be fundamental research tools in many situations and in a variety of environmental conditions, such as the study of biological samples. Among the possible modes of operation, *intermittent contact mode* is one that causes less wear to both the sample and the instrument; therefore, it is ideal when imaging soft samples. However, intermittent contact mode is not particularly fast when compared to other imaging strategies. In this paper, we introduce three enhanced control approaches, applied at both the dither and z-axis piezos that determine the motion of the microscope tip, to address the limitations of existing control schemes. Our proposed practical strategies are able to eliminate different image artefacts, automatically adapt scan speed to the sample being scanned and predict its features in real time. The result is that both the image quality and the scan time are improved.

Index Terms—Atomic force microscope, AFM, intermittent contact mode, IC-AFM, tapping mode, dynamic PID, hybrid PID, scan speed regulator, predictive controller.

I. INTRODUCTION

THE *atomic force microscope (AFM)* is a device with remarkable precision, used to image hard and soft samples at the nanoscale [1]. The microscope senses sample surfaces by means of a flexible cantilever with an atomically-sharp tip at the end. When operated in *intermittent contact mode (IC-AFM, also known as tapping mode)* [2], the cantilever's tip oscillates vertically over the sample surface, driven by a *dither piezo* while the height of the fixed end of the cantilever is manoeuvred by the *z-axis piezo*. As shown in Figure 1, when far away from the sample, the cantilever oscillates at its maximum (or *free*) oscillation amplitude A_f . When the oscillating cantilever comes close to the sample surface, the interaction forces cause the oscillation amplitude A to decrease; a feedback controller adjusts the height $b(t)$ of the base of the cantilever so as to attempt to maintain the current oscillation amplitude $A(t)$ at a constant reference value $A_r < A_f$. The reference amplitude A_r is chosen to balance the need to maximise image quality, while minimising the damage to both the AFM tip and sample resulting from impacts. At the same time, the sample is moved horizontally under the cantilever, generally in a raster pattern, so as to trace the three-dimensional topography of the sample. The oscillation amplitude $A(t)$ is extracted in real time from

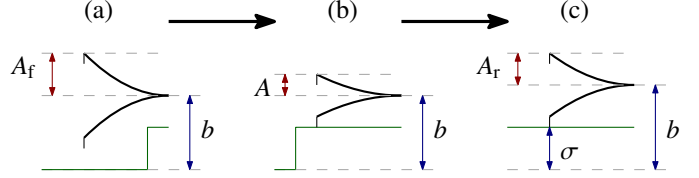


Fig. 1. Operation of an intermittent contact mode AFM. (a) Initially, the flexible cantilever (black curved line) oscillates away from the sample (green), with the free oscillation amplitude A_f . (b) When the distance between the sample surface and the cantilever is reduced, amplitude decreases to a certain value $A < A_f$. (c) Then, a feedback controller regulates the height b of the base of the cantilever so as the oscillation amplitude A reaches the reference value A_r ; this way the cantilever is able to perceive the surface, but impacts very gently once every oscillation period.

the tip position signal, typically measured using the optical beam deflection method [3], operated by a device known as *demodulator*, from which the height of the sample surface can be obtained.

However, although the IC-AFM minimizes damage to the samples while imaging them with great accuracy, the process is hindered by its low speed. As a result, much ongoing research focuses on techniques to reduce the overall scan time (e.g. [4]), and on methods to achieve better image quality. The adoption of such techniques allows to use a higher scan speed while still imaging sample features correctly (e.g. [5, 6]). In this paper, after reviewing the limitation of current control approaches, we present new control schemes to help address these issues. Specifically, these strategies allow us to improve image quality by detecting and managing more kinds of image artefacts with respect to established solutions and by predicting features of the samples, exploiting knowledge of those parts which have already been scanned. Therefore, it is possible to increase scan speed, without worsening image quality. Furthermore, we propose to adapt scan speed dynamically, depending on the characteristics of the sample, allowing for faster scans, with no effect on imaging accuracy.

The rest of the paper is outlined as follows. In Section II we give a detailed explanation of how the IC-AFM works, along with a mathematical formulation. Then, existing control approaches and their disadvantages are discussed. After that, in Section III, original solutions are presented to improve the performance and the scanning speed of the microscope. The novel regulators are validated in Section IV on a set of real test samples. Finally, conclusions are drawn in Section V.

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II. AFM: A BRIEF OVERVIEW

A. Cantilever model

The cantilever tip is the core of an atomic force microscope, it can be modeled as a mechanical point mass *impact oscillator* [7]. Specifically, the model can be given as the hybrid dynamical system

$$\begin{cases} \dot{x}_1 = x_2, \\ \dot{x}_2 = -\omega_n^2 x_1 - \frac{\omega_n}{Q} x_2 + u + F(b + x_1 - \sigma), \end{cases} \quad (1)$$

$$u = D \sin(\omega_d t), \quad (2)$$

when the tip is away from the sample, together with the reset law

$$x_2(t^+) = -r x_2(t^-), \quad x_1(t^+) = x_1(t^-) = \sigma(t) - b(t) \quad (3)$$

that models the impact between the cantilever tip and the sample surface (in terms of a change in state in the infinitesimally short time before and after an impact, at times t^- and t^+ respectively). In the above equations (see Figure 2):

- x_1 is the vertical position of the tip with respect to b ;
- x_2 is its vertical velocity;
- $\omega_n = \sqrt{k/m}$ is the natural (or resonant) frequency of the first flexural mode of the cantilever, with m and k being the mass and the stiffness coefficient of the cantilever, respectively;
- $Q = m\omega_n/c$ is its quality factor, with c being the damping coefficient of the cantilever;
- u represents the action of the dither piezo, with D being its driving amplitude and ω_d its driving frequency;
- F are the interaction forces normalized to mass depending on the distance l between the tip and the sample, where $l = b + x_1 - \sigma$;
- b is the height of the base of the cantilever;
- σ is the height of the sample surface to be measured;
- r is the restitution coefficient.

If the cantilever were infinitely far from the sample, i.e. assuming $F = 0$ and neglecting (4), at steady state the cantilever tip would oscillate in a sinusoidal motion, with

$$x_1(t) = A_f \sin(\omega_d t + \varphi), \quad (4)$$

where φ is a phase shift and the free oscillation amplitude A_f can be computed as

$$A_f = \frac{D}{\left| \omega_n^2 - \omega_d^2 + \frac{\omega_n}{Q} i \omega_d \right|}, \quad (5)$$

where $i = \sqrt{-1}$. In reality, the distance between the cantilever and the sample is finite, therefore $F \neq 0$ and in ideal operation the reset law (4) triggers once every oscillation period, when the tip impacts the sample surface. As a result, under normal working conditions, with only low velocity impacts, the evolution of tip position in time follows a quasi-sinusoidal motion and can be approximated as

$$x_1(t) \approx A(t) \sin(\omega_d t + \varphi(t)), \quad (6)$$

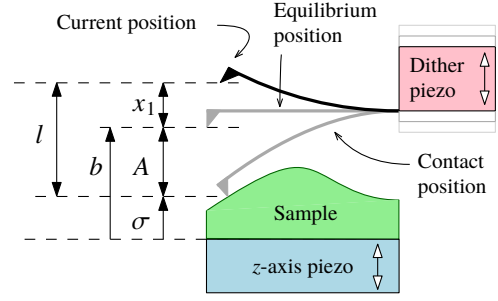


Fig. 2. Schematic representation of the cantilever tip close to the sample surface.

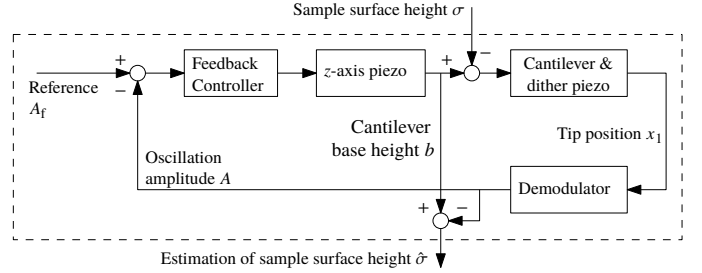


Fig. 3. Block diagram representing the intermittent contact mode atomic force microscope.

with $A(t) \approx b(t) - \sigma(t)$ and $A(t) \leq A_f$.

For what concerns the interaction forces F in (2), we make the approximation that the tip can be modeled as a spherical surface coming in contact with a locally flat sample surface and use the *Derjaguin-Muller-Toporov (DMT) model* [7, 9, 10], so that

$$F(l) = \begin{cases} -\frac{Hr_t}{6l^2}, & l > l_m \\ -\frac{Hr_t}{6l_m^2} + \frac{4}{3} \frac{\sqrt{r_t(l_m - l)^3}}{1 - V_t^2 + \frac{1 - V_s^2}{E_t}} & l \leq l_m \end{cases}, \quad (7)$$

with:

- l being the tip-sample distance;
- H the Hamaker constant;
- r_t the tip radius;
- l_m the intermolecular distance;
- E_t and E_s the elastic moduli of the tip and the sample, respectively;
- V_t and V_s the Poisson ratios of the tip and the sample, respectively.

When the tip and the sample are not too close, there is a small residual attraction between them. However, when the tip-sample distance is reduced below the intermolecular distance l_m repulsive forces dominate and the overall repulsive force becomes larger as l decreases [11].

B. Estimation of the sample surface

For correct operation, the oscillation amplitude A must attain a certain constant reference value A_f , i.e.

$$\lim_{t \rightarrow \infty} A(t) = A_f. \quad (8)$$

TABLE I
PARAMETERS USED FOR THE AFM MODEL, IN ACCORDANCE WITH [7, 8].

Group	Parameter	Value
<i>Cantilever</i>	ω_n	$2.85 \cdot 10^5 \cdot 2\pi$ rad/s
	Q	100
	r	0.9
	k	42 N/m
	$m = k/\omega_n^2$	$1.3098 \cdot 10^{-11}$ kg
	$c = m\omega_n/Q$	$2.3455 \cdot 10^{-7}$ kg/s
<i>Interaction forces</i>	H	$1.4 \cdot 10^{-19}$ J
	r_t	2 nm
	l_m	0.42 nm
	E_t, E_s	$1.65 \cdot 10^{11}$ Pa
	V_t, V_s	0.27
<i>z-axis piezo</i>	ω_{zp}	$1.5 \cdot 10^6 \cdot 2\pi$ rad/s
	Q_{zp}	18
	K_{zp}	$1/\omega_{zp}$
<i>Feedback controller</i>	A_f	variable
	A_r	$0.9A_f$
	K_P, K_D	0
	K_I	10000
	v_x	1 mm/s
<i>Q control</i>	Q'	30
<i>Dynamic/Hybrid PID</i>	K_s	15
	$\Delta Q_{PL}, \Delta Q_{RL}$	25
	A_t^+	$0.95A_f$
	A_t^-	$0.94A_f$
	$A_{t,RL}$	$0.5A_f$
	α_t	$-400A_f$
	τ_v	0.12 ms
<i>Scan speed regulator</i>	$V_{x,0}$	variable
	$V_{x,m}$	$0.1V_{x,0}$
	$V_{x,M}$	$V_{x,0}$
	$b_{M,a}$	$K_I(A_r - A_{t,RL})$
	$b_{M,d}$	$K_I(A_r - A_t^+)$
	$b_{L,a}$	$0.9b_{M,a}$
	$b_{L,d}$	$0.9b_{M,d}$
	$b_{r,a}$	$0.8b_{M,a}$
	$b_{r,d}$	$0.8b_{M,d}$
	M_{PC}	3
<i>Predictive controller</i>	E_σ	$0.1A_f \cdot I_x$
	N_W	$0.01I_x$

This regulation is fundamental, because, if A becomes too small, the interaction forces will damage the sample; whereas, if it becomes too large, the oscillating cantilever tip might easily lose contact with the sample, causing a highly nonlinear and undesirable phenomenon known as *probe loss* or *parachuting*, in which, after the sample surface has decreased rapidly, the cantilever oscillates freely and the measurement is incorrect. Normally, A_r is chosen approximately equal to $0.9A_f$, with the aim of reducing the magnitude of the interaction forces, whose

mean value is proportional to $\sqrt{A_f^2 - A_r^2}$ [2]. A_f is commonly chosen as the smallest value that satisfies $A_f \geq \sigma_{\max} - \sigma_{\min}$, where σ_{\max} and σ_{\min} are the largest and the smallest values of the sample surface height σ on the same scan line (e.g. [7, 12]). However, since σ_{\max} and σ_{\min} are unknown before the scan is performed, A_f has to be selected conservatively, considering the nature of the sample to be imaged.

To ensure (9), a feedback controller is used to adjust b , so that an estimate of surface height σ can be computed as

$$\hat{\sigma} = b - A. \quad (10)$$

Moreover, at the same time, the sample is moved according to a specific pattern on the horizontal x - y plane, so that the whole specimen is imaged. Here we assume that the pattern is a raster one, with the scan lines being parallel to the x -axis. However, the use of more complex patterns, such as spirals, cycloids, and Lissajous has also been proposed with the aim of removing high-frequency components that might excite the actuator's mechanical resonance; see e.g. [2].

A schematic diagram showing the key components needed for estimating the sample surface height is depicted in Figure 3.

C. Existing control approaches

Synthesizing a controller and proving its validity analytically is not trivial. Because of this, a relatively simple scheme such as the PID is a well-established solution to the problem of controlling the cantilever base height b in order to achieve (9) [1]. Moreover, two control schemes named *Q control* [13] and *dynamic PID* [14] are often employed (even together) with the aim of improving the accuracy of the microscope. For the sake of completeness we briefly describe all of these strategies below.

The PID control law is expressed by

$$b(t) = \text{PID}(e_A), \quad (11)$$

where $e_A(t) = A_r - A(t)$ is the error on the oscillation amplitude and the PID control action is the classical one defined as

$$\text{PID}(\xi(t)) = K_P \xi(t) + K_I \int_0^t \xi(\tau) d\tau + K_D \frac{d\xi(t)}{dt}, \quad (12)$$

with K_P , K_I , K_D being constant gains. Nevertheless, since the imaging accuracy given by the PID is typically not sufficient, scan speed cannot be too high. Moreover, this simple regulator does not implement any mechanism to correctly deal with probe loss: a highly nonlinear phenomenon that occurs when the tip and sample lose contact.

The purpose of *Q control* is to mitigate the effect of probe losses by temporarily increasing the speed with which the cantilever reacts. The operation of *Q control* can be understood by considering the cascade of the cantilever and the demodulator as a first order system, in which the input is the dither piezo driving amplitude D , and the state and output is the cantilever oscillation amplitude A [2]; a system with time constant $\tau_A = 2Q/\omega_n$. Therefore, the cantilever can be made more reactive by reducing the effective quality factor Q ,

which, in turn, may be achieved by changing the input from the dither piezo in (3) to

$$u(t) = D \sin(\omega_d t) - K_Q x_2. \quad (13)$$

In so doing, the new effective Q , called Q' , becomes

$$\frac{\omega_n}{Q} + K_Q = \frac{\omega_n}{Q'} \Rightarrow Q' = \left(Q + \frac{K_Q}{\omega_n} \right)^{-1}. \quad (14)$$

Thus, given a desired Q' , the gain of the Q control law must be chosen as

$$K_Q = \omega_n \left(\frac{1}{Q'} - \frac{1}{Q} \right). \quad (15)$$

Furthermore, since A_f depends on Q (see (6)), to avoid changing A_f , a new value D' must be set as

$$D'(Q') = A_f \left| \omega_n^2 + \frac{\omega_n}{Q'} i \omega_d + (i \omega_d)^2 \right|. \quad (16)$$

With the same aim of reducing the detrimental effect of probe losses, the *dynamic PID* addresses the problem of the error e_A saturating to the value $A_r - A_f$. Specifically, the control law (11) is modified as follows. The occurrence of a probe loss is inferred by inspecting the oscillation amplitude A : if it exceeds a threshold $A_t > A_r$, this means that the cantilever is not being limited by proximity with the sample surface and thus a probe loss has occurred. When this happens, part of the error is multiplied by a gain K_s and the control input b is selected according to the switched control law

$$b = \begin{cases} \text{PID}(A_r - A), & A \leq A_t \\ \text{PID}[(A_r - A_t) + K_s(A_t - A)], & A > A_t \end{cases}, \quad (17)$$

where the PID control action is defined as in (12). Typically the threshold A_t is chosen to be slightly larger than A_r [8].

D. Open problems and imaging artefacts

While probe loss is extensively studied in the literature (e.g., [1]), there exist two other subtler image artefacts that can equally deteriorate image quality but are less investigated: we shall term them as *recoil* and *recovery*. Both are illustrated in Figure 4, which shows the result of a numerical simulation that includes both Q control and dynamic PID.

Recoil happens when the sample to be imaged presents a steep upward step (see Figure 4, $t \approx 0.6$ ms). In that case, the cantilever-sample separation $b - \sigma$ suddenly decreases and the interaction forces increase; as a consequence, the oscillation amplitude A decreases quickly to a value smaller than $b - \sigma$ and the oscillating cantilever loses contact with the sample. During this time, the feedback controller is ineffective, because the value of A is not representative of the actual distance between the cantilever and the sample. When the undershoot of A is finished, A returns to depend solely on the current cantilever-sample distance $b - \sigma$ and recoil is completed. The effect of a recoil on surface estimation is an image artefact shaped like a bump, because $\hat{\sigma} = b - A$ is larger if A is smaller, during the undershoot.

Recovery occurs after dynamic PID has brought back the cantilever close to the surface, following a probe loss. In this

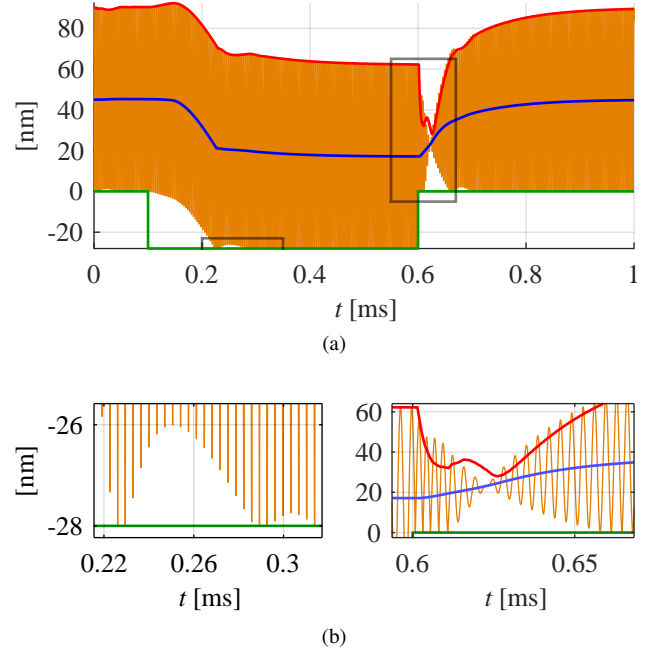


Fig. 4. (a) Scan of an ideal calibration grid, made up of a downward and an upward step, both 28 nm tall, using dynamic PID and Q control; $A_f = 50$ nm. The orange line is the absolute tip position $x_1 + b$; the red line on the top represents $A + b$; the blue line in the middle is the cantilever base height b ; the green line on the bottom is the sample surface height σ . The regions within the black rectangles are magnified in panel (b), where the figure on the left shows recovery in detail, while the one on the right illustrates recoil. The result of these phenomena is that the white space between the orange envelope and the green line is erroneously considered part of the sample surface in the measurement process.

situation there is a very short time in which the regulator keeps decreasing b , even if the cantilever is close to the sample surface; this delay is caused by the finite bandwidth of the feedback controller and the demodulator. As a result the interaction forces cause the oscillation amplitude to decrease to a value smaller than $b - \sigma$, and the cantilever detaches from the sample surface until the undershoot on A finishes. The phenomenon is observable in Figure 4 for $t \approx 0.25$ ms, and the artefact it generates is a false bump, just as for recoil.

Note that neither recoil nor recovery is caused by the presence of the reset law (4). In fact, as Figure 5 shows, the phenomena can happen even when A_f is so small that the reset law is never triggered.

III. IMPROVED AFM CONTROLLERS

In this section, we describe three new practical control schemes designed to overcome the limitations of existing approaches. Firstly, a hybrid PID strategy is used to deal with recovery and recoil, allowing for higher image quality. Secondly, a scan speed regulator is proposed that automatically adapts the scan velocity to the features of the sample, resulting in smaller scan time and greater accuracy. Lastly, a predictive controller is presented that achieves the same result by estimating the upcoming features of the specimen exploiting information obtained from the specimen area that was previously scanned.

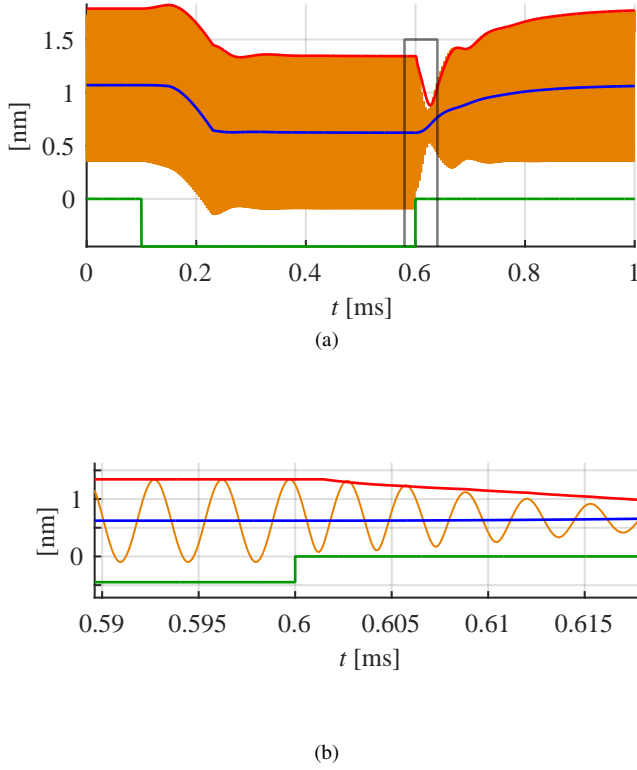


Fig. 5. (a) Scan of an ideal calibration grid with 0.448 nm tall steps, using dynamic PID and Q control; $A_f = 0.8$ nm. The region within the black rectangle is magnified in panel (b), which shows that reset law (4) is never triggered; despite this both recovery and recoil can be seen in panel (a). This is due to the fact that these phenomena depend on the interaction forces F in (2), which can still be felt by the probe, and hence determine the response of the oscillation amplitude A .

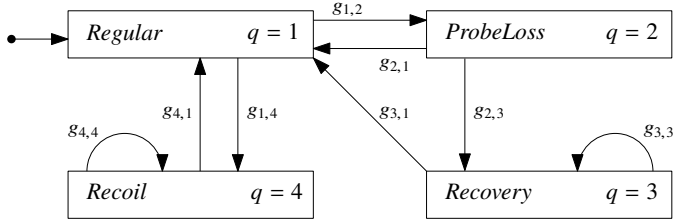


Fig. 6. Hybrid PID scheme. The arrow starting from a black dot represents the initial state. Guards $g_{i,j}$ are described in Table II.

A. Hybrid PID

To address the problems caused by probe losses, recoveries and recoils, we propose a *hybrid PID* strategy which combines the use of the z -axis piezo — which varies b — with the dither piezo — which causes the oscillation of the cantilever. The controller has 4 possible modes, as shown in Figure 6, of which only one is active at any time; the discrete variable $q \in \{1, 2, 3, 4\}$ identifies the current mode. In all modes, the z -axis piezo output is determined by the control law

$$b = \begin{cases} \text{PID}(A_r - A), & A \leq A_t^+ \\ \text{PID}[(A_r - A_t^+) + K_s^q(A_t^+ - A)], & A > A_t^+ \end{cases}, \quad (18)$$

while the dither piezo output is chosen as

$$u = D^q \sin(\omega_d t) - K_Q^q x_2, \quad (19)$$

TABLE II
GUARDS FOR THE TRANSITIONS IN HYBRID PID. BRACES CONTAIN ACTIONS PERFORMED DURING THE TRANSITIONS.

Name	Condition, {action}	Type
$g_{1,2}$	$A \geq A_t^+$	threshold
$g_{2,1}$	$A \leq A_t^-$	threshold
$g_{2,3}$	$\dot{A} < \alpha_t, \{\rho \rightarrow \text{false}; t_0 = t\}$	impact
$g_{3,3}$	$\dot{A} > 0 \wedge \rho = \text{false}, \{\rho \rightarrow \text{true}\}$	wait
$g_{3,1}$	$(\dot{A} < 0 \wedge \rho = \text{true}) \vee (t - t_0 \geq K_\tau \tau_A)$	impact or timeout
$g_{1,4}$	$A \leq A_{t,RL}, \{\rho \rightarrow \text{false}; t_0 = t\}$	threshold
$g_{4,4}$	$\dot{A} > 0 \wedge \rho = \text{false}, \{\rho \rightarrow \text{true}\}$	wait
$g_{4,1}$	$(\dot{A} < \alpha_t \wedge \rho = \text{true}) \vee (t - t_0 \geq K_\tau \tau_A)$	impact or timeout

where variables K_s^q , D^q and K_Q^q depend on the current mode. Normally — i.e. in absence of probe loss, recovery and recoil — *Regular* ($q = 1$) is the active mode. If, at a certain point, a probe loss (with subsequent recovery) or a recoil are detected, the controller switches to a different mode and the behaviors of the piezos change accordingly. Specifically,

$$K_s^q = \begin{cases} 1, & q = 1, 3, 4 \\ K_s, & q = 2 \end{cases}; \quad (20)$$

which simply means that *Regular*, *Recovery* and *Recoil* modes ($q = 1, 3, 4$, respectively) use a regular PID, while *ProbeLoss* mode ($q = 2$) employs a dynamic PID. Also, the mode-dependent control parameters D^q and K_Q^q are defined to be

$$D^q = \begin{cases} D', & q = 1, 2 \\ A_f \left| \omega_n^2 + \frac{\omega_n}{Q_{PL}(A)} i \omega_d + (i \omega_d)^2 \right|, & q = 3 \\ A_f \left| \omega_n^2 + \frac{\omega_n}{Q_{RL}(A)} i \omega_d + (i \omega_d)^2 \right|, & q = 4 \end{cases}, \quad (21)$$

$$K_Q^q = \begin{cases} K_Q, & q = 1, 2 \\ \omega_n \left(\frac{1}{Q_{PL}(A)} - \frac{1}{Q} \right), & q = 3 \\ \omega_n \left(\frac{1}{Q_{RL}(A)} - \frac{1}{Q} \right), & q = 4 \end{cases}, \quad (22)$$

with the probe loss (PL) and recoil (RL) Q values being set as

$$Q_{PL}(A) = Q' - \Delta Q_{PL} \min \left\{ \left| \frac{A_r - A}{A_r - A_f} \right|, 1 \right\}, \quad (23)$$

$$Q_{RL}(A) = Q' - \Delta Q_{RL} \min \left\{ \left| \frac{A_r - A}{A_r - 0} \right|, 1 \right\}, \quad (24)$$

$$\Delta Q_{PL}, \Delta Q_{RL} > 0. \quad (25)$$

That is to say, *Regular* and *ProbeLoss* mode utilize a regular Q control, whereas *Recovery* and *Recoil* modes employ a dynamic damping mechanism, where the further A is from its reference value A_r , the more the cantilever is damped. This is to rapidly extinguish the phenomenon of the undershoot of the oscillation amplitude that happens during recoveries and recoils.

The guards that govern the transitions from one mode to another are reported in Table II and Figure 6, and may be divided into four categories:

- *Threshold conditions.* These are activated when probe losses ($g_{1,2} : A(t) > A_t^+$) and recoils ($g_{1,4} : A(t) < A_{t,RL}$) are detected, and *ProbeLoss* mode ($g_{2,1} : A(t) < A_t^-$) must be exited if a recovery is not detected immediately after probe loss. While probe loss is associated with an excessively large oscillation amplitude, the beginning of recoil is detected when an unusually small amplitude is achieved; therefore, the thresholds have to be set so that $A_t^+ > A_r$ and $A_{t,RL} < A_r$. Moreover, in order to obtain a controller which is less subject to noise on A , A_t^- must be selected so that $A_t^- < A_t^+$, creating a sort of hysteresis between *Regular* and *ProbeLoss* modes.
- *Impact conditions.* These depend on dA/dt and are employed to detect the beginning and end of recovery and the end of recoil. In fact, recovery begins after probe loss when the oscillating cantilever impacts the sample surface ($g_{2,3}$), then the cantilever briefly detaches from the sample and the phenomenon ends after a second impact with the surface ($g_{3,1}$). Similarly, recoil terminates when the cantilever oscillating in free air impacts the sample surface ($g_{4,1}$). A threshold α_t is included in $g_{2,3}$ and $g_{4,1}$ to account for signal noise on dA/dt , whereas it is absent in $g_{3,1}$, where the impact is expected to happen gently and dA/dt is monotone;
- *Wait conditions.* These guards are used as self-loops to remain in *Recovery* ($g_{3,3}$) and *Recoil* ($g_{4,4}$) modes with the purpose of waiting for a change in the sign of dA/dt , in order to allow for the correct detection of impacts; the completion of such event is signalled by the Boolean variable ρ ;
- *Timeout conditions* are set along with the impact conditions in $g_{3,1}$ and $g_{4,1}$ for those cases where impacts are not detected.

B. Scan speed regulator

We present next an additional control scheme aimed at reducing scan time, which can be achieved by employing at all times the largest scan speed that allows for a correct imaging. Ideally, the best way to accomplish this would be to adjust the scan speed v_x dynamically, according to the rate of change of the sample surface, $|d\sigma/dt|$, so that when the latter is large (small), the former is small (large). However, $|d\sigma/dt|$ is not easily measurable, therefore we propose that v_x may be varied depending on the time-derivative db/dt of the z -axis piezo input generated by the PID controller, since, if $|db/dt|$ is large (small), $|d\sigma/dt|$ is likely to be large (small) as well. Furthermore, $|d\sigma/dt|$ is actually a function of v_x , in the sense that if $v_x \rightarrow 0$, the surface height σ does not change under the cantilever and $|d\sigma/dt| \rightarrow 0$ too. Thus, v_x must be set so that $|d\sigma/dt|$ (i.e. $|db/dt|$) is kept within some acceptable range. The thresholds can be chosen considering that, adopting a hybrid PID strategy, the most critical values of db/dt are $b_{M,a} = K_I(A_r - A_{t,RL})$ and $b_{M,d} = K_I(A_r - A_t^+)$. The former, $b_{M,a}$ (“maximum ascending”), is the positive value of db/dt

that, when reached, causes the hybrid PID to switch to *Recoil* mode, whereas the latter, $b_{M,d}$ (“maximum descending”), is the negative value of db/dt that causes the switch to *ProbeLoss* mode. Both should be avoided, in order not to trigger recoil or probe loss. In light of this, a set of four parameters, $b_{L,a}$, $b_{r,a}$, $b_{L,d}$, $b_{r,d}$, have to be selected. Specifically:

- $b_{L,a} < b_{M,a}$ (“limit ascending”) is the positive upper bound for db/dt . The scan speed regulator is set so that db/dt is kept below $b_{L,a}$, in order to ensure $db/dt < b_{M,a}$ at all times;
- $b_{r,a} < b_{L,a}$ (“reference ascending”) is the positive reference value for db/dt attained by the regulator when $db/dt > 0$;
- $b_{L,d} > b_{M,d}$ (“limit descending”) is the negative lower bound for db/dt , with the purpose of guaranteeing $db/dt > b_{M,d}$;
- $b_{r,d} > b_{L,d}$ (“reference descending”) is the negative reference value for db/dt when $db/dt < 0$.

The result is that the parameters are ordered as follows:

$$b_{M,d} < b_{L,d} < b_{r,d} < 0 < b_{r,a} < b_{L,a} < b_{M,a}. \quad (26)$$

We propose to set scan velocity v_x adaptively as the solution of the following first order piecewise-smooth adaptation law:

$$\dot{v}_x = \begin{cases} \frac{1}{\tau_v} \left[-v_x + \left(V_{x,M} - K_{v,a} \left| \frac{db}{dt} - b_{r,a} \right| \right) \right], & \frac{db}{dt} > b_{r,a} \\ \frac{1}{\tau_v} [-v_x + V_{x,M}], & b_{r,d} \leq \frac{db}{dt} \leq b_{r,a} \\ \frac{1}{\tau_v} \left[-v_x + \left(V_{x,M} - K_{v,d} \left| \frac{db}{dt} - b_{r,d} \right| \right) \right], & \frac{db}{dt} < b_{r,d} \end{cases} \quad (27)$$

$$K_{v,a} = \frac{V_{x,M}}{|b_{L,a} - b_{r,a}|}, \quad K_{v,d} = \frac{V_{x,M}}{|b_{L,d} - b_{r,d}|}. \quad (28)$$

Here, $V_{x,M}$ is the (arbitrary or physical) maximum speed of the piezo maneuvering the x -axis and τ_v is a time constant that must be compatible with the time response of the piezo. The difference between the three cases in (27) is the input: it drives v_x to the maximum value $V_{x,M}$ if db/dt is between its reference values $b_{r,d}$ and $b_{r,a}$; otherwise, it reduces v_x all the way down to zero as db/dt approaches $b_{L,a}$ or $b_{L,d}$. However, since for practical reasons it is better not to arrest the piezo completely, a limit is set on minimum velocity as well, so that, at any time,

$$V_{x,m} \leq v_x \leq V_{x,M}. \quad (29)$$

The initial value of the scan speed, $V_{x,0}$, may be set either close to $V_{x,m}$, if there is a desire to act more conservatively and privilege image accuracy, or close to $V_{x,M}$, if a fast scan is the priority. Among the advantages of this control technique is the use of different scan speeds for the ascending and descending parts of the samples, since only the latter threaten probe loss and thus require greater care.

Note that this is by no means the only controller to propose use of the local surface slope; see, for example, [6] — in which it is used to dynamically change the orientation of the oscillation of the tip — and [5] — where it is employed to make a local prediction of the sample features.

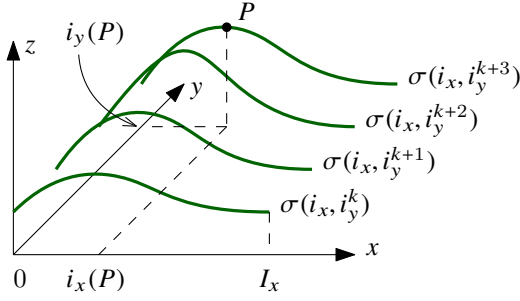


Fig. 7. Representation of scan lines in three-dimensional space.

C. Predictive controller

In the framework of the raster scan pattern, we propose to use a predictive controller to exploit information acquired from previous lines in the scan of the current one. As shown in Figure 7, let

- $i_x(P)$ be the x coordinate of a point P on the sample surface;
- $i_y(P)$ its y coordinate;
- I_x the length of a scan line;
- I_y the length of the sample along the y -axis.

We suggest to extend the PID controller by adding a term to the standard PID regulator (11) of the form

$$b(i_x, i_y^k) = \text{PID}(A_r - A) + \sum_{j=1}^{M_{PC}} K_{\sigma,j} \hat{\sigma}'(i_x, i_y^{k-j}), \quad (30)$$

where the suffix k denotes the coordinate of the k -th raster line. Here, M_{PC} is the number of previous lines used, i.e. the memory horizon of the predictive controller, $\hat{\sigma}'(i_x, i_y^{k-j})$ is a filtered version of the estimation of the $(k-j)$ -th line and $K_{\sigma,j}$ are adaptive gains. Converting information derived from scanned lines into a feedforward action for b is straightforward, because, in a proper scan, b is just a reproduction of σ , with the oscillation amplitude A acting like a cushion to give the feedback controller the necessary time to adjust b to σ . Thus, in this scheme, after the first M_{PC} lines, the role of the PID is not to estimate σ on a line, but to compensate the differences between the past M_{PC} lines and the current one. In Equation (30), the sample surface estimation $\hat{\sigma}'$ is a window-filtered version of the original, i.e.

$$\hat{\sigma}'(i_x, i_y^k) = \frac{1}{2N_W} \int_{i_x - N_W}^{i_x + N_W} \hat{\sigma}(\xi, i_y^k) d\xi. \quad (31)$$

where it is assumed that $\hat{\sigma}(\xi, i_y^k) = \hat{\sigma}(0, i_y^k)$, $\xi \in [-N_W, 0)$ and $\hat{\sigma}(\xi, i_y^k) = \hat{\sigma}(I_x, i_y^k)$, $\xi \in (I_x, I_x + N_W]$. This filtering is necessary because only the general shape of the scan lines is likely to recur in the following ones. In addition, the adaptive gains are selected according to the law

$$K_{\sigma,j} = \begin{cases} \frac{1}{2j} \max \left\{ \frac{E_\sigma - e_{\sigma,j}}{E_\sigma}, 0 \right\}, & j \in [1, M_{PC} - 1] \\ \frac{1}{2(j-1)} \max \left\{ \frac{E_\sigma - e_{\sigma,j}}{E_\sigma}, 0 \right\}, & j = M_{PC} \end{cases}, \quad (32)$$

where

$$e_{\sigma,j} \equiv \int_0^{I_x} \left| \hat{\sigma}'(i_x, i_y^{k-j}) - \hat{\sigma}'(i_x, i_y^{k-j-1}) \right| di_x. \quad (33)$$

Note that the gains $K_{\sigma,j}$ are normalized by the factors $1/2j$ and $1/2(j-1)$, so that their sum is, at the most, unity. Moreover, the more recent a line (smaller j), the higher the coefficient. The results of the “max” operations span from 0 to 1. In particular, when $e_{\sigma,j}$, which represents how much a line is different from the previous one, is equal to or greater than a threshold E_σ , the result is 0. Hence, the line is too different from the previous one to be used as a predictive tool and the gain $K_{\sigma,j}$ is set to zero, switching off the predictive term in the controller (30).

IV. NUMERICAL VALIDATION

A. Settings and Samples

To validate the new control strategies, we make the following assumptions regarding the AFM:

- The dynamics of the dither piezo are much faster than that of the system, i.e. the largest time constant of the former is significantly smaller than $1/\omega_n$;
- The z -axis piezo can be modeled as a second order system [8], with gain K_{zp} , natural frequency ω_{zp} and quality factor Q_{zp} (see Table I).
- Q control is always employed and tip velocity x_2 is assumed measurable.

Validation will be performed on five samples: two ideal, purely numerical ones, and three real ones, previously acquired with a custom built contact mode high-speed AFM at the University of Bristol Centre for Nanoscience and Quantum Information Low Noise Labs.

These are:

- An ideal calibration grid, with 28 nm tall steps and a spatial period of 1 μm , with each period having one downward and one upward step;
- A real titanium disulfide sample (see Figure 8a);
- An ideal quasi-sinusoidal sample, which is the sum of a sine having a spatial period of 4 μm and an amplitude of 80 nm and a triangular waveform having amplitude and period each a tenth of those of the sine;
- A real calibration grid sample (see Figure 8b);
- A real uranium oxide sample (see Figure 8c).

All simulations were run in Matlab Simulink [15], using Stateflow toolbox that uses an event-driven solver to simulate the reset law (4) correctly. This is coupled with a variable-step Dormand-Prince (ode45) solver, with maximum step size 10^{-7} , minimum step size 10^{-13} and relative tolerance 10^{-4} . In addition, all parameters which are not expressed explicitly are taken from Table I, unless stated otherwise.

B. Validation of hybrid PID

Figure 9 represents the scan of the ideal calibration grid, performed with a hybrid PID. Compare it with Figure 4, where the classical dynamic PID is used on the same sample: in the former, the bump at time $t \approx 0.25$ ms, associated with the recovery phenomenon, has practically disappeared; also,

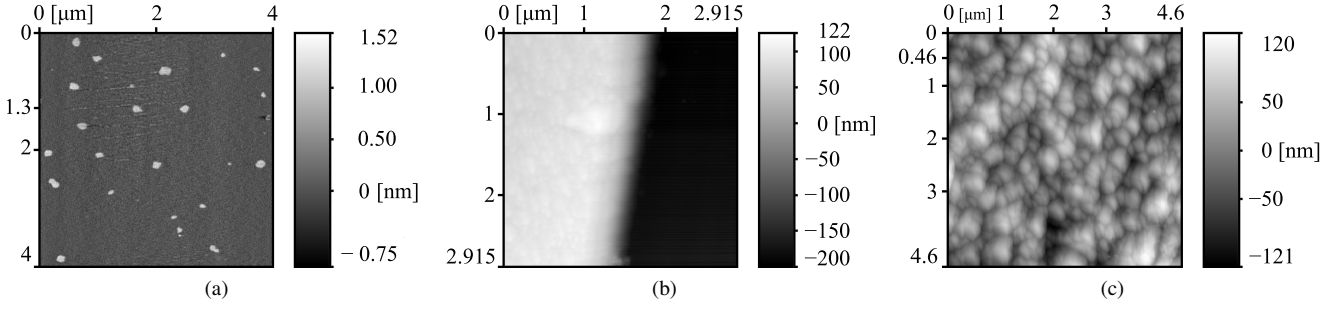


Fig. 8. (a) Sample of titanium disulfide, provided by Chris Howard (University College London); (b) Veeco Instruments (now Bruker) calibration grid; (c) sample of uranium oxide, produced by Anna Adamska (University of Bristol).

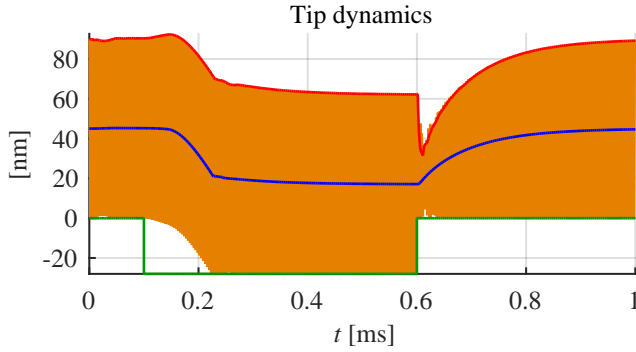


Fig. 9. Scan of the ideal calibration grid with hybrid PID; $A_f = 50$ nm.

recoil decays much faster when employing the hybrid PID. Note that the dynamics of the z -axis piezo, represented as the blue line in Figures 4 and 9, does not change significantly, because it depends on the gains K_P , K_I , and K_D which are not varied in the *Recovery* and *Recoil* modes. Table III reports the results of four different cases of scans of a 10-periods-long ideal calibration grid. In the table, the variable $e_{\sigma, \max}^{RV}$ indicates the maximum height of the bump observed during a recovery. The comparison between the third rows in the first two sub-tables shows that the hybrid PID reduces the root mean square value of $e_{\sigma, \max}^{RV}$ by 58.9%. Furthermore, the fact that the impact velocity v_i — i.e. the value of x_2 when the reset law is triggered — does not increase points out that the new controller achieves this result without increasing the effect of the interaction forces. The third case shows that a hybrid PID that uses *Recoil* mode gives an error 6.5% smaller than that of an hypothetical hybrid PID that does not employ it. However, if the error is computed only during recoils, where the mode is active, the error reduction is about 20%. Finally, a similar result is represented in the fourth case, with noise on the position signal x_1 , having a magnitude that is 1% that of A_f and $\alpha_t = -600A_f$ (while in absence of noise $\alpha_t = -400A_f$).

Figures 10a and 10b report the surface estimations of the titanium disulfide sample on the scan line corresponding to $i_y = 1.3 \mu\text{m}$ when using the dynamic PID and the hybrid PID, respectively. Table IV reports quantitative findings, showing that the root mean square error decreases by 18.2%, when using the new scheme.

TABLE III

RESULTS OF SCANS OF A 10-PERIOD-LONG IDEAL CALIBRATION GRID. e_{σ} [nm] IS THE ESTIMATION ERROR; v_i [mm/s] IS THE IMPACT VELOCITY, I.E. WHEN (4) TRIGGERS; $e_{\sigma, \max}^{RV}$ [nm] IS THE HEIGHT OF THE BUMP IN A RECOVERY. RMS IS THE ROOT MEAN SQUARE VALUE AND SD IS THE STANDARD DEVIATION.

Case	Variable	RMS	SD	Max
1. <i>Dynamic PID</i>	e_{σ}	8.27	8.61	28.09
	v_i	11.78	10.12	-74.40
	$e_{\sigma, \max}^{RV}$	2.04	0.77	3.33
2. <i>Hybrid PID w/o Recoil mode</i>	e_{σ}	8.26	8.64	28.08
	v_i	11.60	9.94	-74.34
	$e_{\sigma, \max}^{RV}$	0.84	0.48	1.69
3. <i>Hybrid PID</i>	e_{σ}	7.72	8.21	28.09
	v_i	11.38	9.68	-74.48
	$e_{\sigma, \max}^{RV}$	1.33	0.65	2.12
4. <i>Hybrid PID with noise</i>	e_{σ}	7.88	7.96	28.18
	v_i	10.07	8.69	-74.33
	$e_{\sigma, \max}^{RV}$	0.92	0.30	1.35

TABLE IV

RESULTS OF SCANS OF THE TITANIUM DISULFIDE SAMPLE.

Case	Variable	RMS	SD	Max
1. <i>Dynamic PID</i>	e_{σ}	0.22	0.22	0.98
	v_i	0.76	0.24	-1.10
2. <i>Hybrid PID</i>	e_{σ}	0.18	0.19	0.86
	v_i	0.76	0.24	-1.09

C. Validation of scan speed regulator

When scanning the ideal quasi-sinusoidal sample with constant scan speed $v_x = 1$ mm/s and using the hybrid PID, the AFM is not able to image the sample properly and probe losses happen during the descending part of the surface, as shown in Figure 11a. Instead, a nearly perfect scan is achieved when adding the scan speed regulator, with $V_{x, M} = V_{x, 0} = 1$ mm/s and $V_{x, m} = V_{x, 0}/10$, as depicted in Figure 11b (see also Figure 11c). The comparison between the sub-tables in Table V shows that, when using the scan speed regulator, the root mean square

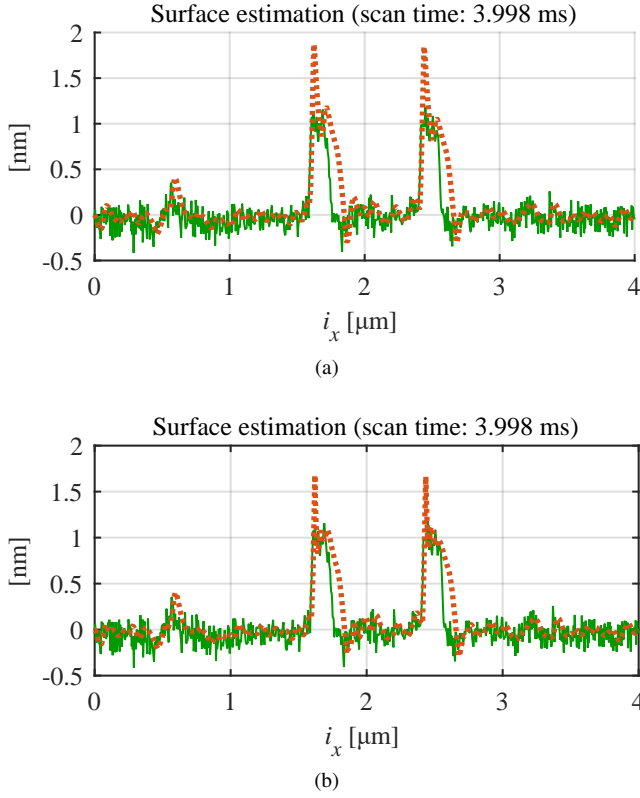


Fig. 10. Surface estimations of the titanium disulfide sample with (a) dynamic PID and (b) hybrid PID; scan line $i_y = 1.3 \mu\text{m}$, $A_f = 2 \text{ nm}$. The green solid line is the real sample surface height σ and the orange dotted line is the estimated sample surface height $\hat{\sigma}$.

TABLE V
RESULTS OF SCANS OF THE SINUSOIDAL SAMPLE. T_s [ms] IS THE SCAN TIME.

Case	Variable	RMS	SD	Max
1. Hybrid PID ($v_x = 1 \text{ mm/s}$)	e_{σ}	1.66	1.66	8.24
	v_i	5.88	2.88	-19.77
	T_s	3.998	-	-
2. Hybrid PID and speed regulator	e_{σ}	0.23	0.25	2.01
	v_i	4.09	2.02	-19.77
	T_s	8.591	-	-
3. Hybrid PID ($v_x = 0.421 \text{ mm/s}$)	e_{σ}	0.24	0.25	1.79
	v_i	4.25	1.91	-16.84
	T_s	9.501	-	-

error decreases by 86%. To obtain the same level of accuracy without the scan speed regulator, it would be necessary to reduce the scan speed to $v_x = 0.421 \text{ mm/s}$, as in case 3, having however the scan time increased by 10.6% with respect to case 2. For the sake of completeness, Figure 12 shows the evolution of v_x and db/dt with and without scan speed regulator, corresponding to the scans shown in Figure 11.

To further validate these findings, compare the results of a scan of the first line ($i_y = 0 \mu\text{m}$) of the real calibration grid without the scan speed regulator, reported in Figure 13a, with

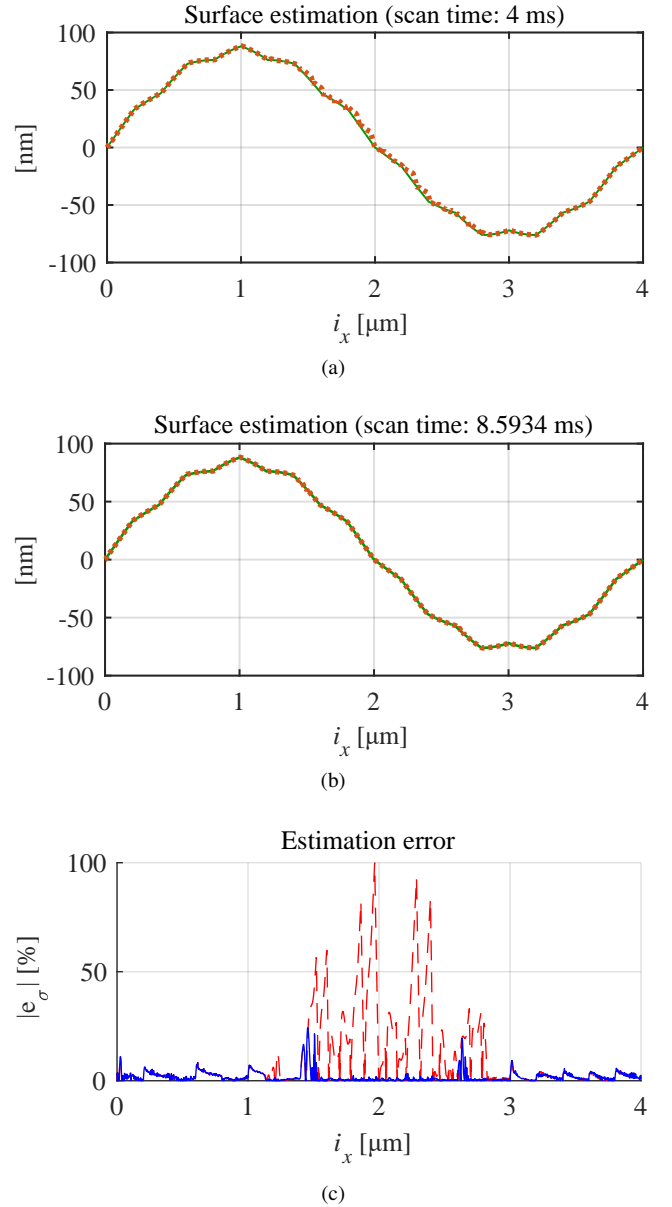


Fig. 11. Surface estimations of the sinusoidal sample with (a) hybrid PID ($v_x = 1 \text{ mm/s}$) and with (b) hybrid PID and scan speed regulator; $A_f = 50 \text{ nm}$. The green solid line is the real sample surface height σ and the orange dotted line is the estimated sample surface height $\hat{\sigma}$. (c) Percentage of the absolute value of the estimation errors e_{σ} in the cases with hybrid PID (dashed red line) and with hybrid PID and scan speed regulator (solid blue line); 100% corresponds to the maximum error of the hybrid PID, 8.24 nm.

a scan performed while employing it, depicted in Figure 13b; quantitative results are in Table VI. In particular, when using the scan speed regulator the error decreases by 47% and the scan time by 3%.

D. Validation of predictive controller

The predictive controller has been tested together with the scan speed regulator on the uranium oxide sample; Figure 14 depicts a scan of the whole surface, which may be compared with the original in Figure 8c. In addition, the results of a series of comparative tests are reported in Table VII. In these simulations the first 100 lines of the sample are scanned ($i_y =$

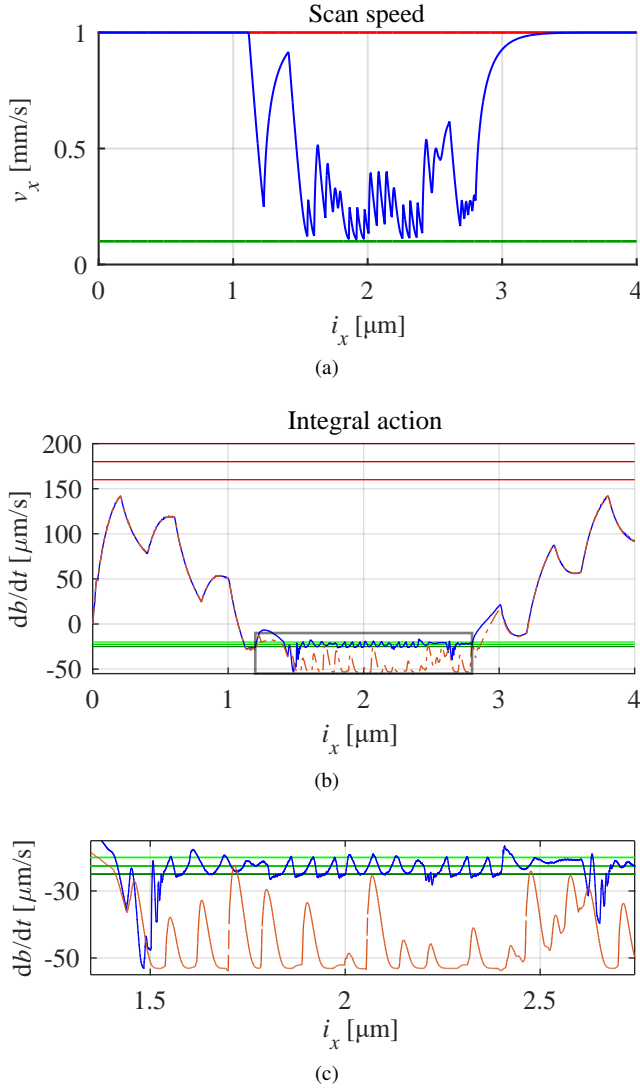


Fig. 12. (a) Scan speed v_x relative to the scan in Figure 11b. The blue line is v_x , the red line on the top is $V_{x,M}$ and the green line on the bottom is $V_{x,m}$. (b) Integral action db/dt relative to the scans in Figures 11a and 11b. The three lines on the top in shades of red are $b_{M,a}$, $b_{L,a}$ and $b_{r,a}$, recalling that $b_{M,a} > b_{L,a} > b_{r,a}$. The three lines on the bottom in shades of green are $b_{M,d}$, $b_{L,d}$ and $b_{r,d}$, with $b_{M,d} < b_{L,d} < b_{r,d}$. The dashed orange line is the integral action relative the scan in Figure 11a (w/o speed regulator), whereas the blue solid line is the integral action relative to the scan in Figure 11b (w/ speed regulator). The region within the black rectangle is magnified in panel (c), illustrating a detail corresponding to the descending part of the sample.

0 μm to $i_y = 0,46 \mu\text{m}$), in four different configurations, given by the possible combinations of the predictive controller and the scan speed regulator. In a scenario where the scan speed regulator is not used, adding the predictive controller reduces the error by 39.4% (cases 1 and 2). In contrast, when using an AFM which implements the speed regulator, the predictive controller reduces the error by 18.6% and the scan time by 19.9% (cases 3 and 4). In conclusion, comparing the results given by the four configurations, the best solution is to employ the predictive controller together with the scan speed regulator, in order to have the best accuracy, reduced scan time and self-selection of scan speed.

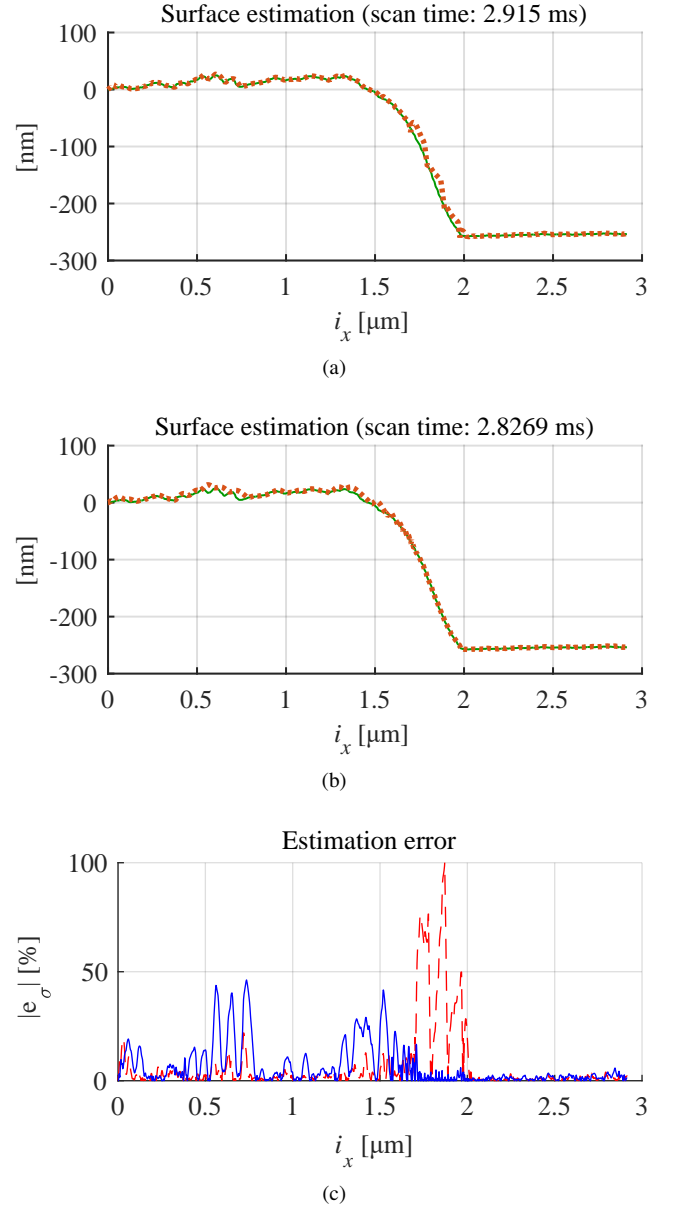


Fig. 13. Surface estimations of the real calibration grid using (a) the hybrid PID ($v_x = 1 \text{ mm/s}$) and (b) the hybrid PID and the scan speed regulator ($V_{x,0} = 2 \text{ mm/s}$); scan line $i_y = 0 \mu\text{m}$, $A_f = 300 \text{ nm}$. The green solid line is the real sample surface height σ and the orange dotted line is the estimated sample surface height $\hat{\sigma}$. (c) Percentage of the absolute value of the estimation errors e_σ in the cases with hybrid PID (dashed red line) and with hybrid PID and scan speed regulator (solid blue line); 100% corresponds to the maximum error of the hybrid PID, 30.26 nm.

V. CONCLUSIONS

In this paper we have introduced three original controllers that achieve two fundamental goals: improving the accuracy and reducing the scan time of the intermittent contact mode atomic force microscope. Firstly, a hybrid PID scheme was introduced which is able to deal with image artefacts such as recoils and recoveries. Secondly, an adaptive scan speed regulator is proposed to set scan speed dynamically, depending on the characteristics of the sample surface. As a result, scan time decreases, accuracy being equal. Finally, a predictive controller is used to improve both the image quality and the

TABLE VI
RESULTS OF SCANS OF THE REAL CALIBRATION GRID.

Case	Variable	RMS	SD	Max
1. <i>Hybrid PID</i> ($v_x = 1$ mm/s)	e_σ	5.43	5.76	30.26
	v_i	29.66	13.86	-107.49
	T_s	2.915	-	-
2. <i>Hybrid PID and speed regulator</i> ($V_{x,0} = 2$ mm/s)	e_σ	2.88	2.98	15.05
	v_i	29.98	14.75	-91.30
	T_s	2.827	-	-

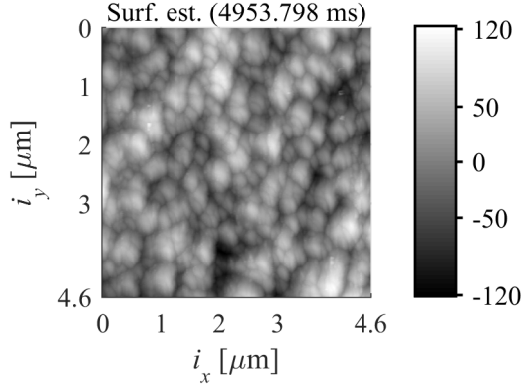


Fig. 14. Surface estimation of the uranium oxide sample with hybrid PID, scan speed regulator and predictive controller; $A_f = 200$ nm.

scan time, exploiting information from previously scanned lines in the imaging of the current one.

Further research will focus on the experimental implementation of the proposed strategies and the investigation of the implications of the use of the presented controllers in combination with the most recent developments, such as *multifrequency AFM* [16], which would require more detailed models of the cantilever dynamics.

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TABLE VII
RESULTS OF SCANS OF URANIUM OXIDE. T_s [ms] IS THE SCAN TIME OF A SINGLE LINE AND $T_{s,tot}$ [ms] IS THE TOTAL SCAN TIME.

Case	Variable	Mean	Max
1. <i>w/o predictive controller, w/o speed regulator</i>	$RMS(e_\sigma)$	5.82	7.79
	$SD(e_\sigma)$	5.06	6.87
	K_σ	0.000	0.000
	T_s	4.600	4.600
	$T_{s,tot}$	460.000	-
2. <i>w/ predictive controller, w/o speed regulator</i>	$RMS(e_\sigma)$	3.53	5.83
	$SD(e_\sigma)$	2.83	5.01
	K_σ	0.886	0.927
	T_s	4.600	4.600
	$T_{s,tot}$	460.000	-
3. <i>w/o predictive controller, w speed regulator</i>	$RMS(e_\sigma)$	4.06	5.58
	$STD(e_\sigma)$	3.56	4.95
	K_σ	0.000	0.000
	T_s	6.248	6.810
	$T_{s,tot}$	624.770	-
4. <i>w/ predictive controller, w speed regulator</i>	$RMS(e_\sigma)$	3.31	4.50
	$STD(e_\sigma)$	2.71	3.96
	K_σ	0.888	0.927
	T_s	5.004	6.455
	$T_{s,tot}$	500.359	-



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